

# Hybrid theory of *P*-wave electron-hydrogen elastic scattering

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We report on a study of electron-hydrogen scattering, using a combination of a modified method of polarized orbitals and the optical potential formalism. The calculation is restricted to *P* waves in the elastic region, where the correlation functions are of Hylleraas type. It is found that the phase shifts are not significantly affected by the modification of the target function by a method similar to the method of polarized orbitals and they are close to the phase shifts calculated earlier by Bhatia [Phys. Rev. A 69, 032714 (2004)]. This indicates that the correlation function is general enough to include the target distortion (polarization) in the presence of the incident electron. The important fact is that in the present calculation, to obtain similar results only 35-term correlation function is needed in the wave function compared to the 220-term wave function required in the above-mentioned previous calculation. Results for the phase shifts, obtained in the present hybrid formalism, are rigorous lower bounds to the exact phase shifts.

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## I. Introduction

Scattering of electrons by hydrogenic systems is always of interest because the target function is known exactly, allowing us to test the various methods of calculation. At low incident energies, the distortion of the target produced by the incident electron is important. One of the methods used to take into account this distortion is the method of polarized orbitals [1], which includes the effect of polarization and essential physics in the ansatz for the scattering wave function. Various other approximations have been used: Kohn-Feshbach variational method [2], Kohn variational method [3], *R*-matrix method [4], and the finite element method [5]. In previous papers [6, 7], the *P*-wave e-H and e-He<sup>+</sup> scattering phase shifts were calculated by using the Feshbach projection operator formalism [8]. The results obtained are accurate and have variational lower bounds. But it has not been possible to take into account in the Feshbach formalism the distortion produced by the incident electron which results in a direct  $-1/r^4$  potential in the scattering equation.

In [9], the *S*-wave electron-hydrogen scattering phase shifts were calculated by using a hybrid method in which both long-range potential proportional to  $-1/r^4$  and short-range correlations via an optical potential were included in the scattering equation at the same time. We did not use any projection operators in this calculation [9] but the important property, namely, that the phase shifts are rigorous lower bounds to the exact phase shifts, is retained [10]. We follow the same procedure in the present calculation on

$P$ -wave scattering as in [9]. We use Rydberg units: energy in Rydbergs and length in Bohr radius  $a_0$ .

## II. Theory

The total spatial wave function for e-H partial wave (denoted by  $L$ ) problem is written as

$$\Psi_L(\vec{r}_1, \vec{r}_2) = \frac{u_L(r_1)}{r_1} Y_{L0}(\hat{r}_1) \phi_0(r_2) \pm (1 \leftrightarrow 2) + \sum_{\lambda}^N C_{\lambda} \Phi_L^{\lambda}(\vec{r}_1, \vec{r}_2) \quad (1)$$

$N$  is the number of terms in the expansion. The target wave function is given by

$$\phi_0(r_2) = (Z^3 / \pi)^{0.5} e^{-Zr_2}, \quad (2)$$

where  $Z$  is the charge of the nucleus. The  $(\pm)$  above refers to singlet (upper sign) or triplet (lower sign) scattering, respectively. Beyond the terms containing  $u_L$  explicitly (those are the terms giving rise to the exchange approximation), the functions  $\Phi_L$  are the correlation functions. These functions include all the many-body effects and the scattering equation is a single-particle equation. For arbitrary  $L$  this function is most efficiently written in terms of the Euler angles [11]:

$$\Phi_L = [f_L^{\kappa+}(r_1, r_2, r_{12}) D_L^{\kappa+}(\vartheta, \phi, \psi) + f_L^{\kappa-}(r_1, r_2, r_{12}) D_L^{\kappa-}(\vartheta, \phi, \psi)] \quad (3)$$

The  $D^{\kappa, \varepsilon}$  functions ( $\varepsilon = +1, -1$ ) are called *rotational harmonics* [11] and are functions of the Euler angles  $\vartheta, \phi, \psi$ . The  $f$ 's above are generalized “radial” functions which depend on the three residual coordinates that are required (beyond the Euler angles) to define the two vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . The distance between two electrons is  $r_{12} = |\vec{r}_1 - \vec{r}_2|$ . The radial functions are defined as follows

$$f_1^{1+} = \cos(\vartheta_{12} / 2) [f(r_1, r_2, r_{12}) \pm f(r_2, r_1, r_{12})], \quad (4)$$

$$f_1^{1-} = \sin(\vartheta_{12} / 2) [f(r_1, r_2, r_{12}) \mp f(r_2, r_1, r_{12})], \quad (5)$$

$\vartheta_{12}$  is the angle between  $\vec{r}_1$  and  $\vec{r}_2$ , and

$$f(r_1, r_2, r_{12}) = \sum_{lmn} C_{lmn} r_1^l r_2^m r_{12}^n e^{-\gamma r_1 - \delta r_2} \quad (6)$$

The minimum value of  $l$  is equal to 1 while that of  $m$  and  $n$  is 0. First, we derive the wave function of the scattered electron **without the long-range correlations** and it is given implicitly by

$$\int [Y_{10}^*(\Omega_1)\phi_0^*(\vec{r}_2)(H-E)\Psi_L]d\vec{r}_2 = 0, \quad (7)$$

$H$  is the Hamiltonian and  $E$  is the total energy of e-H scattering system:

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{2}{r_{12}}, \quad (8)$$

$$E = k^2 - Z^2, \quad (9)$$

$k^2$  is the kinetic energy of the incident electron and  $Z=1$  is the nuclear charge which is equal to 1 in the present calculation (electron-hydrogen scattering).

In order to derive the equation eq. (7) for the scattering function  $u(r_1) \equiv u_L(r_1)$ , the coefficients  $C_\lambda$  must be known. Taking  $N=1$ , for illustration, we calculate the functional (arising in the Kohn variational principle)

$$I = \langle \Psi_L(\vec{r}_1, \vec{r}_2) | H - E | \Psi_L(\vec{r}_1, \vec{r}_2) \rangle, \quad (10)$$

which can be written as

$$I = A + C_1 B + C_1^2 D, \quad (11)$$

where

$$A = \langle [\phi_0(\vec{r}_2)u(\vec{r}_1) \pm (1 \leftrightarrow 2)] | H - E | [\phi_0(\vec{r}_2)u(\vec{r}_1) + (1 \leftrightarrow 2)] \rangle, \quad (12)$$

and

$$B = 2 \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | [\phi_0(r_2)u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle = 4 \langle V_1(r_1)u(r_1) \rangle, \quad (13)$$

where

$$V_1(r_1) = \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \phi_0(\vec{r}_2)Y_{10}(\Omega_1) \rangle, \quad (14)$$

and

$$D = \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) \rangle = \varepsilon_1 - E, \quad (15)$$

$\varepsilon_1$  is the expectation value of  $H$ ,

$$\langle \Phi_L^{(1)} | H | \Phi_L^{(1)} \rangle = \varepsilon_1, \quad (16)$$

and  $\Phi_L^{(1)}$  is normalized to unity. The variation with respect to  $C_1$ , i.e.,

$$\frac{\partial I}{\partial C_1} = 0, \quad (17)$$

implies

$$B + 2C_1D = 0. \quad (18)$$

This gives

$$C_1 = -\frac{B}{2D} = \frac{4 \langle \Phi_L^{(1)}(\vec{r}_1, \vec{r}_2) | H - E | \phi_0(r_2) Y_{10}(\Omega_1) \rangle}{H - \varepsilon_1} = \frac{2 \langle V_1(r_1) u(r_1) \rangle}{E - \varepsilon_1}. \quad (19)$$

The equation for the scattering function can be obtained from  $\frac{\delta I}{\delta u} = 0$ , which reduces to

$$\langle Y_{10}(\Omega_1) \phi_0(\vec{r}_2) | H - E | \Psi_L \rangle = 0, \quad (20)$$

and this can be simplified to

$$\langle Y_{10}(\Omega_1) \phi_0(\vec{r}_2) | H - E | [\phi_0(\vec{r}_2) u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle + C_1 \langle Y_{10}(\Omega_1) \phi_0(\vec{r}_2) | H - E | \Phi_L^{(1)} \rangle = 0, \quad (21)$$

or

$$\langle Y_{10}(\Omega_1) \phi_0(\vec{r}_2) | H - E | [\phi_0(\vec{r}_2) u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle + C_1 V_1(r_1) = 0, \quad (22)$$

Where  $V_1(r_1)$  is given in Eq. (14). Substitution of  $C_1$  from Eq.(19) into Eq.(22) gives the equation

$$\langle Y_{10}^*(\Omega_1) \phi_0(\vec{r}_2) | H - E | [\phi_0(\vec{r}_2) u(\vec{r}_1) \pm (1 \leftrightarrow 2)] \rangle + \frac{2V_1(r_1) \langle V_1(r) u(r) \rangle}{E - \varepsilon_1} = 0 \quad (23)$$

The resulting equation for  $u_L(r)$  can be written in the form

$$\left[ \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + V_d \pm V_{ex} - V_{op} + k^2 \right] u_L(r) = 0, \quad (24)$$

where

$$V_{op}u_L = 2r \sum_{\lambda=1}^N \frac{V_{\lambda}(r) \langle V_{\lambda}(r_1)u(r_1) \rangle}{E - \varepsilon_{\lambda}}. \quad (25)$$

In [6, 7], the optical potential of the type given in Eq. (24) was derived by using the Feshbach projection operator formalism [8] based on projection operators  $\mathbf{P}$  and  $\mathbf{Q}$ . The present formalism is independent of the projection operators  $\mathbf{P}$  and  $\mathbf{Q}$ .

In the above formalism [6, 7], those terms coming from the correlation function are such that they take into account only the short-range correlations and there is no direct long-range potential proportional to  $1/r^4$  in the scattering equation satisfied by  $u(r)$ .

### III. Optical potential with polarization

This long-range potential is due to the polarization of the target wave produced by the presence of the incident electron. This can be taken into account by the method of polarized orbitals. Temkin [12] has shown, using the adiabatic approximation in the first-order theory and using the dipole part of the resulting perturbed wave function, that in the presence of the incident electron  $r_1$ , the effective target wave function can be written as

$$\Phi^{pol}(\vec{r}_1, \vec{r}_2) = \phi_0(\vec{r}_2) - \frac{\chi_{\beta}(r_1)}{r_1^2} \frac{u_{1s \rightarrow p}(r_2)}{r_2} \frac{\cos(\vartheta_{12})}{\sqrt{Z\pi}}, \quad (26)$$

where

$$u_{1s \rightarrow p}(r_2) = e^{-Zr_2} \left( \frac{Z}{2} r_2^3 + r_2^2 \right), \quad (27)$$

and  $\vartheta_{12}$  is the angle between  $\vec{r}_1$  and  $\vec{r}_2$ . We have replaced the step function  $\varepsilon(r_1, r_2)$  used by Temkin [12] by a smooth cutoff function  $\chi_{\beta}(r_1)$  which is of the form

$$\chi_{\beta}(r_1) = (1 - e^{-\beta r_1})^n, \quad (28)$$

where  $n \geq 3$ . Now the polarization takes place whether the scattered electron is inside or outside the orbital electron. The polarization function given in Eq. (26) is valid throughout the range. This is unlike the step function  $\varepsilon(r_1, r_2)$  used by Temkin [12] which ensures that the polarization takes place when the scattered electron  $r_1$  is outside the orbital electron  $r_2$ . Furthermore, the function in Eq. (28) gives us another nonlinear parameter  $\beta$ , which is a function of  $k$ , the incident electron momentum, along with the exponent  $n$ . This term guarantees that  $\chi_{\beta}(r_1)/r_1^2 \rightarrow 0$  when  $r_1 \rightarrow 0$  and it also contributes to the short-range correlations in addition to those obtained from the

correlation function  $\Phi_L$ , and therefore, is useful to optimize the results. Now the electron-target wave function can be written as

$$\Psi_L(\vec{r}_1, \vec{r}_2) = \frac{u_L(r_1)}{r_1} Y_{L0}(\Omega_1) \Phi^{pol}(\vec{r}_1, \vec{r}_2) \pm (1 \leftrightarrow 2) + \sum_{\lambda} C_{\lambda} \Phi_L^{\lambda}(\vec{r}_1, \vec{r}_2) \quad (29)$$

We arrive at the same form of the scattering equation as Eq. (24), when we replace  $\phi_0(\vec{r}_2)$  by  $\Phi^{pol}(\vec{r}_1, \vec{r}_2)$  given in Eq. (26). We further restrict ourselves to  $L=1$  and we can write the final equation in the form

$$[D(r) \frac{d^2}{dr^2} + k^2 + \frac{2}{r^2} + V_d + V^{pol} \pm (V_{ex} + V_{ex}^{pol}) - V_{op}^{pol}] u(r) = 0. \quad (30)$$

We give below various quantities:

$$D(r) = 1 + \frac{43}{8Z^6} \left( \frac{\chi_{\beta}(r)}{r^2} \right)^2. \quad (31)$$

The direct potentials are given by

$$V_d = \frac{2(Z-1)}{r} + 2e^{-2Zr} \left( Z + \frac{1}{r} \right), \quad (32)$$

and

$$V_d^{pol} = (x_1 + x_3) + x_2 \frac{d}{dr}, \quad (33)$$

We give  $x_1$ ,  $x_2$  and  $x_3$  below

$$x_1 = 2 \frac{\chi_{\beta}(r)}{(Zr)^4} \alpha(r) \quad (34)$$

$$\alpha(r) = \frac{9}{2} - \frac{2}{3} e^{-2Zr} (1.5(Zr)^4 + 7.5(Zr)^3 + 13.5(Zr)^2 + 13.5(Zr) + 6.75) \quad (35)$$

$$x_2 = B_1(r) \frac{43}{4Z^6} \left( \frac{\chi_{\beta}(r)}{r^2} \right)$$

$$x_3 = -\frac{9}{2} \left( \frac{\chi_{\beta}(r)}{Z^2 r^2} \right)^2 + 43(B_2(r) + \frac{2Z}{r} - \frac{4}{r^2} + k^2) \frac{\chi_{\beta}(r)}{8Z^6 r^2} - d(r) \frac{\chi_{\beta}(r)}{Z^5 r^4} \quad (36)$$

$$B_1(r) = (n\beta e^{-\beta r} (1 - e^{-\beta r})^{n-1} - \frac{2\chi_\beta(r)}{r}) / r^2 \quad (37)$$

$$B_2(r) = n\beta e^{-\beta r} (Bx(r) + By(r)) / r^2 + 2(\frac{\chi_\beta(r)}{r^4} - \frac{B_1(r)}{r}) \quad (38)$$

$$Bx(r) = -(\beta + 2/r)(1 - e^{-\beta r})^{n-1} \quad (39)$$

$$By(r) = \beta e^{-\beta r} (n-1)(1 - e^{-\beta r})^{n-2} \quad (40)$$

$$d(r) = \frac{43}{4Zr} + \frac{48}{(Zr)^3} - e^{-2Zr} (0.5(Zr)^4 + 4.5(Zr)^3 + 18(Zr)^2 + 45(Zr) + 81.25 + dxx) \quad (41)$$

$$dxx = \frac{106.75}{(Zr)} + \frac{96}{(Zr)^2} + \frac{48}{(Zr)^3} \quad (42)$$

It can be seen that  $(x_1 + x_3)$  has a term

$$\frac{9}{2Z^4 r^4}, \quad (43)$$

where  $9/(2Z^4)$  is the dipole polarizability of the target with nuclear charge  $Z$ . In addition to this term, there are other terms proportional to  $1/r^2$ ,  $1/r^3$ , and  $1/r^4$  in the direct potential. They go to zero for  $r \rightarrow 0$ . The exchange terms are given by

$$V_{ex} u(r) = -\frac{8Z^3}{3} e^{-Zr} \left[ \frac{1}{r} \int_0^r dx e^{-Zx} x^2 u(x) + r^2 \int_r^\infty dx \frac{e^{-Zx}}{x^2} u(x) \right], \quad (44)$$

The exchange polarization terms are too detailed and are not given here. The optical potential is given by

$$V_{op}^{pol} u(r) = r \sum_s^N \frac{\langle Y_{10}^*(\Omega_1) \Phi^{pol}(\vec{r}_1, \vec{r}_2) | H - E | \Psi_0' \rangle}{E - \varepsilon_s}, \quad (45)$$

where  $\Psi_0'$  is the wave function  $\Psi_0$  given in Eq. (29) without the correlation term  $\Phi_L$ .

This Optical potential includes the effects of polarization. The right hand side of Eq. (45) has not been given explicitly because it contains a large number of terms.

## IV. Calculation and Results

Eq. (30) is solved for the continuum function  $u_l$  by the noniterative method of Omidvar [13] and the phase shift  $\eta$  is obtained from the value of the function at large distance:

$$\lim_{r \rightarrow \infty} u_l(r) \propto \sin(kr - l\frac{\pi}{2} + \eta). \quad (46)$$

In order to obtain phase shifts which can be compared to those obtained by the method of polarized orbitals, we exclude the correlation terms  $\Phi_L$  in Eq. (1). Also, the present cutoff function  $\chi_\beta$  given in Eq. (36), which allows optimization with respect to  $\beta$  to get the best results, is replaced by the cutoff function obtained by Shertzer and Temkin [14]:

$$\chi_{ST} = 1 - e^{(-2Zr)} \left[ \frac{(Zr)^4}{3} + \frac{4(Zr)^3}{3} + 2(Zr)^2 + 2(Zr) + 1 \right] \quad (47)$$

Now the calculation should be similar to that carried out by the method of polarized orbitals. The results obtained by the use of two different cutoffs are not very different. The phase shifts obtained, using this cutoff of Shertzer and Temkin [14], for  $^1P$  and  $^3P$  are given in Table I. and compared with those obtained by Sloan [15]. These results include contributions from the exchange polarization terms. The present results have variational bounds, i.e., they are always lower than the exact phase shifts. We see that phase shifts, obtained using the polarized orbital method, are always higher than the present ones.

In Table II, we give the convergence of  $^1P$  phase shifts for  $k=0.1$  with increasing number of terms in the correlation function. We use the cutoff function given in Eq. (28). The results have been optimized with respect to the nonlinear parameters  $\beta$ ,  $\gamma$  and  $\delta$ , with  $n=3$ , the optimum value. We see that we do not need more than 35 terms to get results comparable to those obtained in [6] without the use of the polarization term in the target wave function and using the Feshbach formalism of projection operators, where it is not possible to modify the formulation in such a way as to produce a direct polarization potential proportional to  $1/r^4$  in the scattering equation.

Gailitis [16] has shown that as the number of terms in the correlation function is increased the optical potential become more attractive. Consequently, phase shifts increase as the number of terms is increased. We see from the results given in Table II that this holds true.

In Table III, we give  $^1P$  phase shifts for values of the incident momentum from  $k=0.1$  to 0.8 for 35 terms and compare them with those obtained in [6] with 220 terms in the correlation function, but without the polarization term. We see that in most case the results are comparable in accuracy to those obtained previously [6] with longer expansions in the correlation function. This indicates that very long expansions do give



fairly accurate results. We also compare the present results with the variational results of Ajmera and Chung [17], *R*-matrix results of Scholz *et al.* [4] and the finite element results of Botero and Shertzer [5]. Most of the results are comparable but the results obtained in [4, 5, 16] for  $k=0.4$  to  $0.8$  are rather too low compared to the present results. The phase shifts obtained in the above-mentioned calculations do not have any variational bounds. It should be noted that the phase shifts increase up to  $k=0.3$  and then start decreasing up to  $k=0.7$  and increase again.

In Table IV, we give the convergence of  $^3P$  phase shifts for  $k=0.1$  with the number of terms in the correlation function. Again, we use the cutoff function given in Eq. (28). The results have been optimized with respect to the nonlinear parameters  $\beta$ ,  $\gamma$  and  $\delta$ , with  $n=3$ , the optimum value. We again see that we do not need more than 35 terms to get results comparable in accuracy to those obtained in [6] without the use of the polarization term in the target wave function and using the Feshbach formalism of projection operators.

In Table V, we give results  $^3P$  phase shifts for values of the incident momentum from  $k=0.1$  to  $0.8$  for 35 terms and compare them with those obtained in [6] with 220 terms in the correlation function, but without the polarization tem. We see that in most case the results are comparable in accuracy to those obtained previously [6] with longer expansions. This indicates that very long expansions do give fairly accurate results because of completeness in the whole space. We also compare the present results with the Kohn variational results of Armstead [18], *R*-matrix results of Scholz *et al.* [4] and the finite element results of Botero and Shertzer [5]. Most of the present results are comparable with the results obtained [4, 5, 14]. It should be noted that the phase shifts for  $^3P$  increase continuously throughout the range from  $k=0.1$  to  $k=0.8$ . Although the differences are small, the present  $^{1,3}P$  are the largest of the lower bound results and therefore are the best.

## V. Low energy scattering

It is known [19] that at low energies  $L=1$  scattering, the long-range correlations contribute most to the phase shift:

$$\tan(\eta)/k^2 = \pi\alpha/15 - Ak. \quad (48)$$

So that

$$(\tan(\eta(k_1))/k_1^2 - \tan(\eta(k_2))/k_2^2) = -A(k_1 - k_2). \quad (49)$$

The first term in Eq. (48) is due to the long-range potential and the second term has contributions from the short-range correlations of which there are contributions from the cross of  $\Phi^{pol}$  and  $\Phi_L$  terms. Thus the values of  $A$  of the present calculation do not coincide with values obtained in our previous calculation [6] which included only the short-range correlations. Using phase shifts given in Table VI, we find

$$A^T = -1.002 \text{ and } A^S = 2.942. \quad (50)$$

O'Malley *et al.* [18] obtained  $A(\text{triplet}) \approx -1.3$  and  $A(\text{singlet}) \approx 1.6$  by fitting the phase shifts of the original polarized orbitals calculation (e-H) of Temkin and Lamkin [20]. But the latter calculation, although of historical importance, did not give precision results. Thus, I believe, the  $A$  values obtained in the present calculation are more accurate.

## VI. Conclusions

In conclusion, we have applied the hybrid theory, in the presence of an optical potential, in which the long-range and short-range correlations, as in Eq. (29), can be taken into account at the same time. The close-coupling formalism with short-range correlations is like the present formalism, in the sense that the  $P$  states give the polarizability of the lower-lying  $S$ -state of the target. The  $P$ -wave phase shifts are much more sensitive to polarization and short-range correlations than  $S$ -wave phase shifts [7]. The present results are calculated variationally and therefore have lower bounds to the exact phase shifts. The present results are very close to those obtained in [6], using the Feshbach formalism in which it was not possible to define the projection operators  $\mathbf{P}$  and  $\mathbf{Q}$  to modify the target function to include the effect of the distortion produced by the incident electron. Moreover, shorter expansions of the order of 35 terms are needed to get results comparable in accuracy to those obtained in [6].

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## References

- [1] A. Temkin, Phys. Rev. **107**, 1004 (1957).
- [2] E. McGreevy and A. L. Stewart, J. Phys. B **10**, L527 (1977).
- [3] D. H. Oza, Phys. Rev. A **33**, 824 (1986).
- [4] T. Scholz, P. Scott and P. G. Burke, J. Phys. B **21**, L139 (1986)
- [5] J. Botero and J. Shertzer, Phys. Rev. A **46**, R1155 (1992).
- [6] A. K. Bhatia, Phys. Rev. A **69**, 032714 (2004).
- [7] A. K. Bhatia, Phys. Rev. A **73**, 012705 (2006).
- [8] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).
- [9] A. K. Bhatia, Phys. Rev. A **75**, 032713 (2007).
- [10] P. G. Burke, A. J. Taylor, and S. Ormonde, Proc. Phys. Soc. (London) **92**, 345 (1967).
- [11] A. K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 10-50 (1964).
- [12] A. Temkin, Phys. Rev. Phys. Rev. **116**, 358 (1959).
- [13] K. Omidvar, Phys. Rev. **133**, A970 (1964).
- [14] J. Shertzer and A. Temkin, Phys. Rev. A. **74**, 052701 (2006).
- [15] I. H. Sloan, Proc. Roy. Soc. **281**, 151 (1964).
- [16] M. Gailitis, Soviet Phys. JETP **20**, 107 (1965).
- [17] M. P. Ajmera and K. T. Chung, Phys. Rev. A **10**, 1013 (1974).
- [18] R. L. Armstead, Phys. Rev. **171**, 91 (1968).
- [19] T. F. O'Malley, L. Rosenberg, and L. Spruch, Phys. Rev. **125**, 1300 (1962).
- [20] A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1961)

Table I. Comparison of phase shifts  $\eta$  without correlations with those obtained in [16]

$k$	$^1P$		$^3P$	
	$\eta$	$\eta_{PO}$	$\eta$	$\eta_{PO}$
0.1	0.0057	0.0067	0.0094	0.0109
0.2	0.0110	0.0171	0.0384	0.0486
0.3	0.0006	0.0210	0.0867	0.1151
0.4	-0.0090	0.0163	0.0148	0.2005
0.5	-0.0295	0.0064	0.2100	0.2867
0.6	-0.0495	-0.0039	0.2625	0.3574
0.7	-0.0646	-0.0100	0.2999	0.4063
0.8	-0.0721	-0.0095	0.3225	0.4351

[16] I. H. Sloan, Proc. Roy. Soc. **281**, 151 (1964).

Table II. Convergence of  $^1P$  phase shifts  $\eta$  for  $k=0.1$  with the number of terms.

$N$	B	$\Gamma$	$\delta$	$\eta$
0	0.47			0.0060892
4	0.27	0.42	0.99	0.0062066
10	0.21	0.30	0.99	0.0063271
20	0.34	0.33	0.84	0.0063444
35	0.34	0.30	0.87	0.0063508

Table III. Singlet  $P$  phase shifts  $\eta$  for various  $k$  for  $N=35$

$k$	H	$\eta_{PQ}^a$	$\eta_{AC}^b$	$\eta_{RM}^c$	$\eta_{FEM}^d$
0.1	0.00635076	0.0063083	0.005782	0.006	0.006
0.2	0.01506556	0.014988	0.01445	0.015	0.0148
0.3	0.01670634	0.016613	0.01550	0.016	0.0160
0.4	0.01015347	0.0099980	0.00846	0.009	0.0090
0.5	-0.00061223	-0.00084017	-0.00287	-0.002	-0.0020
0.6	-0.01009367	-0.010359	-0.013029	-0.012	-0.0117
0.7	-0.01321557	-0.013483	-0.017225	-0.016	-0.0149
0.8	-0.00490138	-0.0048524	-0.009544		-0.0068

<sup>a</sup>Phase shifts obtained using the Feshbach formalism [8].

<sup>b</sup>Variational results of Ajmera and Chung [17].

<sup>c</sup> $R$ -matrix results of Scholz *et al.* [4].

<sup>d</sup>Finite element method results of Betero and Shertzer [5].

Table IV. Convergence of triplet  $P$  phase shifts  $\eta$  for  $k=0.1$  with the number of terms.

$N$	B	$\Gamma$	$\delta$	Phase shift
0	0.45	0.35	0.80	0.0098336
4	0.45	0.35	0.80	0.0099701
10	0.45	0.35	0.85	0.0103265
20	0.45	0.37	0.85	0.0103714
35	0.38	0.30	0.80	0.0103813

Table V. Triplet  $P$  phase shifts  $\eta$  for various  $k$  for  $N=35$

$k$	H	$\eta_{PQ}^a$	$\eta_{Kh}^b$	$\eta_{RM}^c$	$\eta_{FEM}^d$
0.1	0.01038234 <sup>e</sup>	0.010382	0.0101	0.010	0.0100
0.2	0.04536735	0.045345	0.0448	0.045	0.0452
0.3	0.1069312	0.10679	0.1059	0.107	0.1067
0.4	0.1888873	0.18730	0.1866	0.187	0.1873
0.5	0.2709762	0.27058	0.2700	0.270	0.2708
0.6	0.3416749	0.34128	0.3405	0.341	0.3417
0.7	0.3932100	0.39257	0.3918	0.392	0.3933
0.8	0.4277296 <sup>e</sup>	0.42730	0.425		0.4283

<sup>a</sup>Phase shifts obtained using the Feshbach formalism [8].

<sup>b</sup>Kohn variational results obtained by Armstead [18].

<sup>c</sup> $R$ -matrix results of Scholz *et al.* [4].

<sup>d</sup>Finite element method results of Botero and Shertzer [5].

<sup>e</sup>Phase shifts for  $k=0.1$  and  $0.8$  are for 56 terms.

Table VI. Low energy  $P$ -wave phase shifts for  $N=35$  and values of  $A$  from the effective range theory.

State	$k_1=0.04$	$k_2=0.05$	$A$
$^1P$	0.001303692	0.001963464	2.942
$^3P$	0.001564346	0.002469346	-1.002

